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Variable Weight Fractional Collisions for Multiple Species Mixtures

Robert Martin

In-Space Propulsion Branch,
Air Force Research Laboratory,
Edwards Air Force Base, CA USA

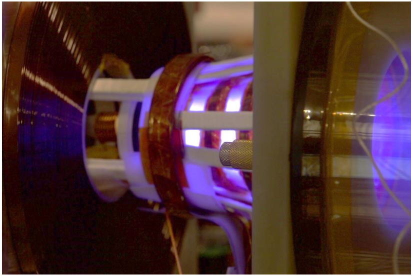
Direct Simulation Monte Carlo, 2017

Outline

Field-Reversed Configuration:

- Concept from Fusion Energy
  - Scaled Down for Propulsion

RP3X FRC Thruster



Field-Reversed Configuration:

- Concept from Fusion Energy
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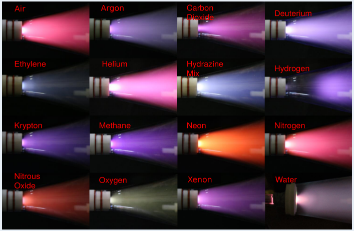
- Electrodeless
  - Limits Erosion
  - Enables Flexible Fuels



Pancotti, et al, "Adaptive Electric Propulsion for ISRU Missions", 20th Adv. Space Prop., 11/2014

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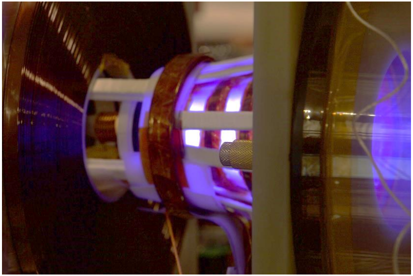

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  - Tunable Thrust/ISP
  - Coupled Dynamics

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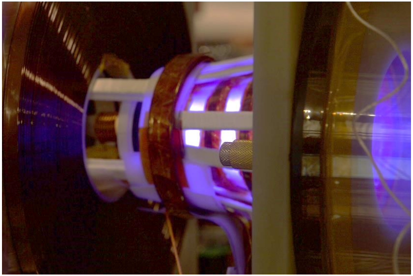

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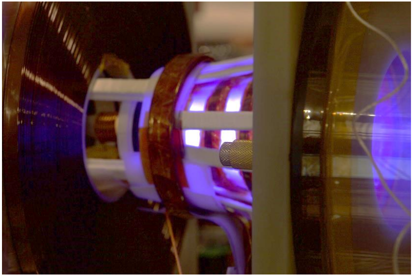

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Complex to Design

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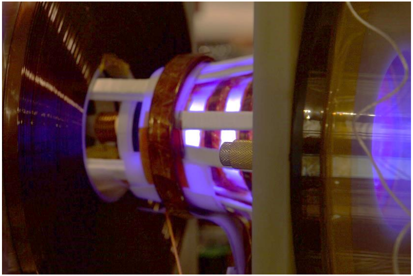

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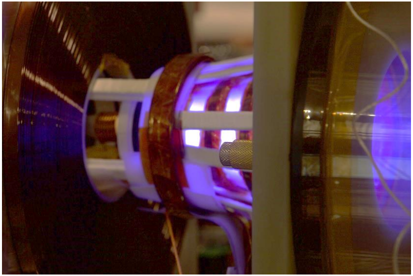
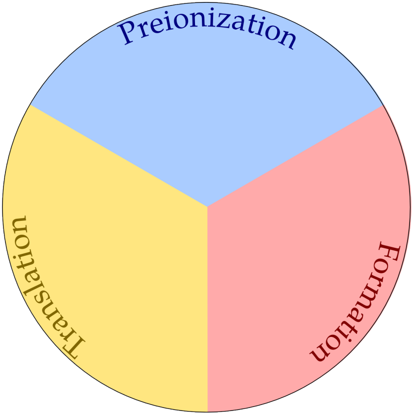
Complex to Design
Significant Modeling Challenge

RP3X FRC Thruster



Dominant Physics Varies with Cycle:



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Dominant Physics Varies with Cycle:

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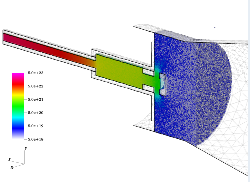
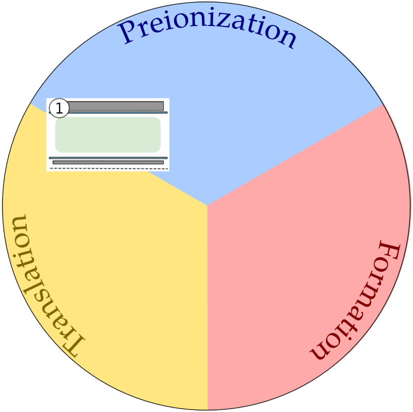
   - Rarefied Kinetic Flow





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Dominant Physics Varies with Cycle:

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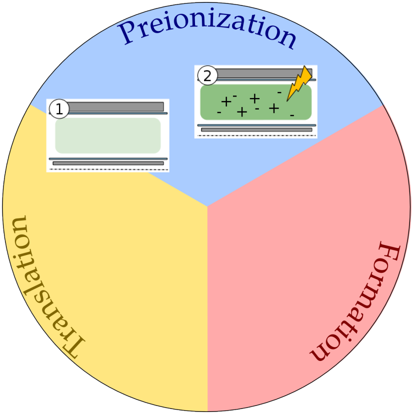

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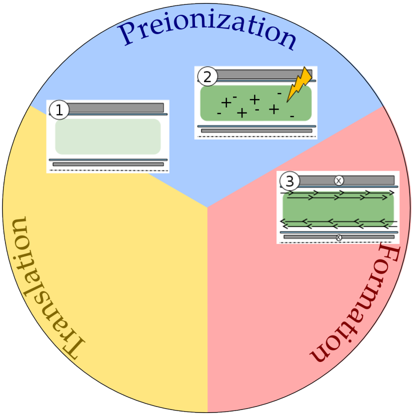
   - Ionization+Electromagnetics



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Phases of FRC Operation

Dominant Physics Varies with Cycle:

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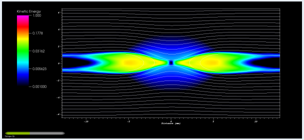
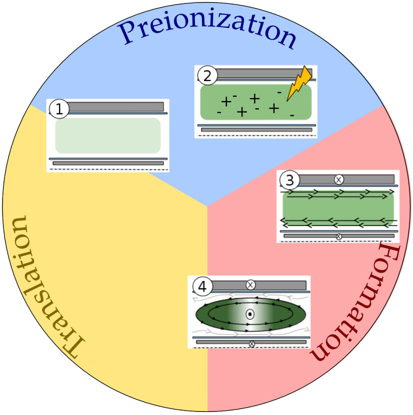


https://astrobear.pas.rochester.edu/trac/wiki/AstroBearProjects/resistiveMHD



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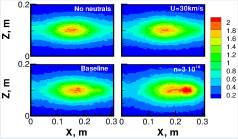
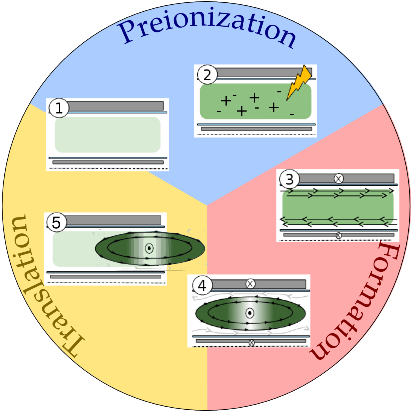
   - $\vec{j} \times \vec{B}$, Neutral Entrainment





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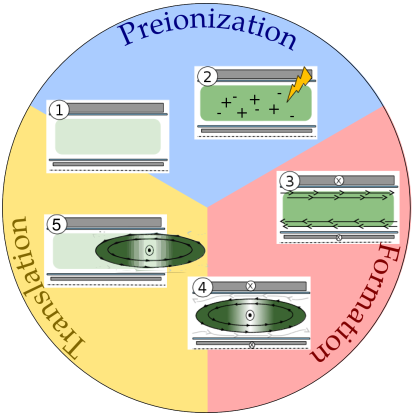
Continuous Cycle: 5 impacts 1



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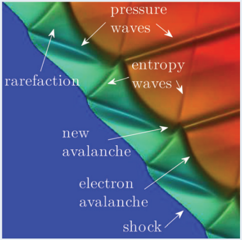
Important Collisions in Spacecraft Propulsion:

- Discharge and Breakdown in FRC
- Collisional Radiative Cooling/Ionization
- Combustion Chemistry

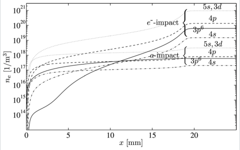
Common Features in Spacecraft Collisions:

- Relevant Densities Spanning Many Orders of Magnitude — 6+
- Transitions from Collisional to Collisionless
- Tiny Early e^- or Radical Populations Critical to Induction Delay
- Many types of Inelastic Collisions with Unknown Effects on Distribution Shapes

Shock Ionization



Kapper & Cambier, J. Appl. Phys. 109, (2011)



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Need Low Noise & High Dynamic Range Collision Algorithms

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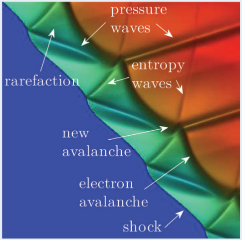

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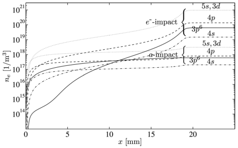


STANDARD COLLISION MODELS

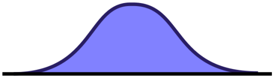
Previous Collision Methods:

- Monte Carlo Collisions (MCC)
  - Particles Collide with Background “Fluid”
  - Often Used in Plasma/PIC Simulation
  - Ion-e^- Collisions Assume Stationary Ions
  - No Conservation/Detailed Balance
- Direct Simulation Monte Carlo Collisions (DSMC)
  - Most Modern Versions use No-Time Counter (NTC) Method
  - Conservative/Reversible Collision
  - Satisfies Detailed Balance
  - Subset of Possible Collisions Sampled
  - Random Selection vs Z_{ij} for All/Nothing Collision

All Random Flip vs Number of Collisions: $Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle$ dt

Continuum to Discrete Representation:

- Many Particles $\xrightarrow{\sim}$ Continuous Distribution



Continuum to Discrete Representation:

- Many Particles $\overset{\sim}{\rightarrow}$ Continuous Distribution
- Discretized VDF Yields Vlasov
  But Collision Integral Still a Problem

Variable Weights for Dynamic Range

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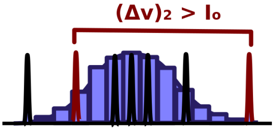

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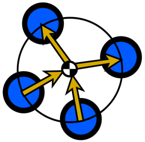
Variable Weight "All-or-Nothing" Collisions?



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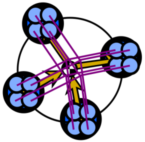

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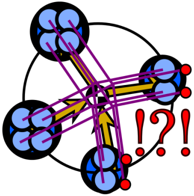
Variable Weight "All-or-Nothing" Collisions?
Physically Inconsistent!
(Mixing Violates Momentum/Energy Conservation)



SWPM Collisions

Stochastic Weighted Particle Method:

- Developed by Rjasanow & Wagner

Attempted Collisions/Cell:

$$\nu = f(2\bar{w} - w_{min}) N_p (N_p - 1) \langle \sigma v \rangle^{max} dt$$

Select Pair (i,j) if:

$$\texttt{Rand} < \frac{w_i + w_j - w_{min}}{N_p (N_p - 1)(2\bar{w} - w_{min})}$$

-or-

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Collide If:

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Perform Standard VHS Collisions

Generate/Modify Particles with:

$$\pm \Delta w / f = \pm \texttt{min}(w_i, w_j) / f$$

Update $\langle \sigma v \rangle^{max}$

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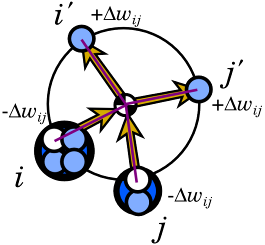

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- Still Requires Merge $w_i \neq \mathtt{const}$

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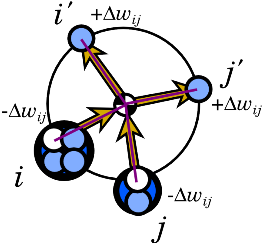


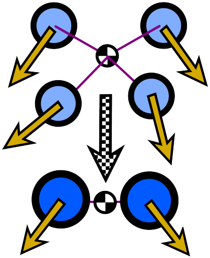
Generate/Modify Particles with:

$$\pm\Delta w/f = \pm\mathtt{min}(w_i, w_j)/f$$

Update $\langle\sigma v\rangle^{max}$

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF



$$w_{cell} = \sum_i^{(n+2)} w_i$$
$$\vec{\bar{v}} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \vec{v}_i$$
$$\overline{V^2} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \left(\vec{v}_i - \vec{\bar{v}}\right)^2$$

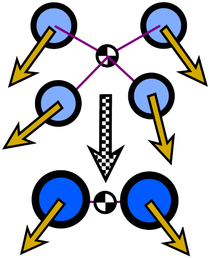
$$w_{(a/b)} = w_m/2$$
$$\vec{v}_{(a/b)} = \vec{\bar{v}} \pm \hat{\mathcal{R}}\sqrt{\overline{V^2}}$$

Similarly: $\vec{x}_{(a/b)} = \vec{\bar{x}} \pm \hat{\mathcal{R}}\sqrt{\overline{X^2}}$

Merge to Pair $\rightarrow$ DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

Selection of Near Neighbors in VDF Limits Thermalization



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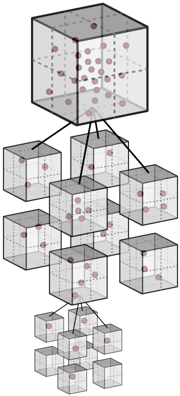
Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

Selection of Near Neighbors in VDF Limits Thermalization

Merge via Separate Octree/Species
Only Change for Mixtures!

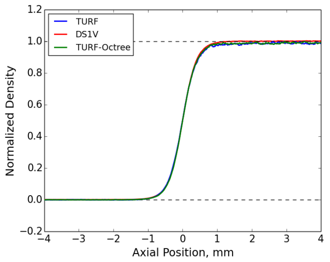
Octree Velocity Bins



Efficient Neighbor Selection

1D Normal Argon Shock Test

- Simple Verification vs. DS1V
- Initial Conditions:
  $T_0 = 293\text{K}$, $n_0 = 1\text{E}22/\text{m}^3$, $v_0 = 637.4(\text{m/s})$
- Initial Jump to Post-Shock at 1cm
- VHS Collisions:
  T_{ref}=273K, d_{ref}=4.17Å, ω_{VHS}=0.81



1D Normal Argon Shock Test

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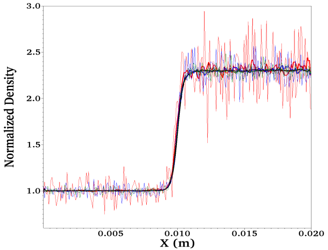
- Time Average:
  $\bar{n}$ from t$\in [80, 100)\mu$s

TURF - SWPM+Octree



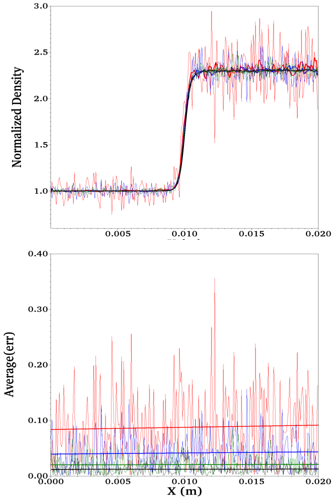
Target N/Cell Quadrupled per Line

From RGD30: Mach 2 Argon Shock

1D Normal Argon Shock Test

- Simple Verification vs. DS1V
- Initial Conditions:
  $T_0 = 293\text{K}$, $n_0 = 1\text{E}22/\text{m}^3$, $v_0 = 637.4(\text{m/s})$
- Initial Jump to Post-Shock at 1cm
- VHS Collisions:
  T_{ref}=273K, d_{ref}=4.17Å, ω_{VHS}=0.81
- Time Average:
  $\bar{n}$ from t$\in [80, 100)\mu$s
- Error (Normalized L_1):
  $err = |n - \bar{n}|/\bar{n}$
- Error Controlled: $err \propto \sqrt{N/cell}$

TURF - SWPM+Octree

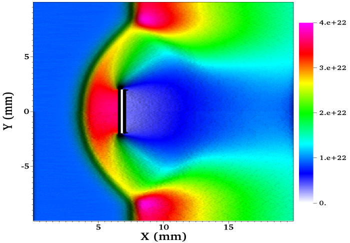


Target N/Cell Quadrupled per Line

2D Argon Shock Test

- Initial Conditions like M=2 Except: $v_0 = 2550\text{m/s}$
- Specular: x=5 − 5.04mm with y=±2mm
- Half Domain Modeled: $80\mu\text{m} \times 80\mu\text{m}$ Cells

TURF: n - Standard DSMC



TURF: n - SWPM+Octree

2D Argon Shock Test

- Initial Conditions like M=2 Except:
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- Specular: x=5 − 5.04mm with y=±2mm
- Half Domain Modeled:
  80μm × 80μm Cells
- Time Average:
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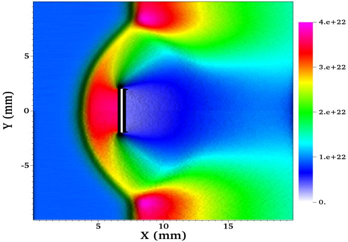
- SWPM Similar to Standard DSMC

TURF: n - Standard DSMC

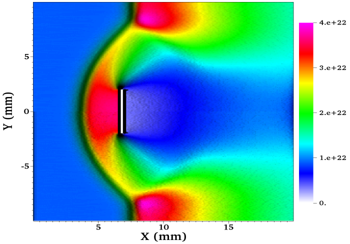


TURF: n - SWPM+Octree

2D Argon Shock Test

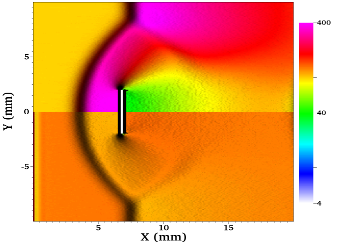
- Initial Conditions like M=2 Except: $v_0 = 2550$m/s
- Specular: x=5 − 5.04mm with y=±2mm
- Half Domain Modeled: 80μm × 80μm Cells
- Time Average: $\bar{n}$ from t$\in[80, 100)\mu$s
- SWPM Similar to Standard DSMC
- Despite Different $Np/Cell$

TURF: n - Standard DSMC



TURF: n - SWPM+Octree

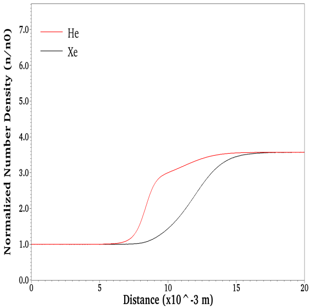
TURF Np/Cell - Standard DSMC



TURF Np/Cell - SWPM+Octree

1D Normal He:Xe Shock Test

- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)



Converged 100x Baseline

1D Normal He:Xe Shock Test

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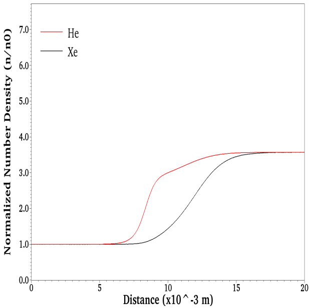
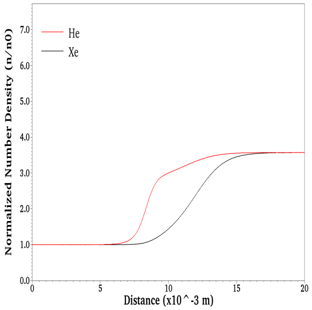
- Highlights Species Separation



Converged 100x Baseline

1D Normal He:Xe Shock Test

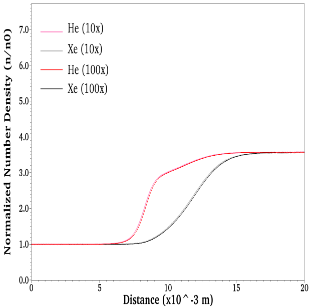
- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)
- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$



Converged 100x Baseline

1D Normal He:Xe Shock Test

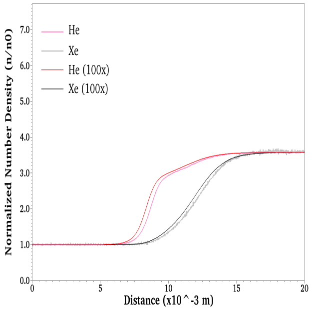
- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)
- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error



Comparison 10x vs. 100x

1D Normal He:Xe Shock Test

- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)
- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error
- Error in Time Average at Baseline

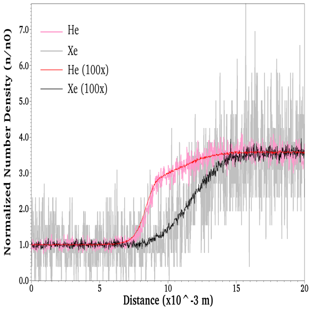


Comparison Baseline vs. 100x

He:Xe Mixture Shock

1D Normal He:Xe Shock Test

- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)
- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error
- Error in Time Average at Baseline
- Instantaneous: Dramatic Noise in Xe

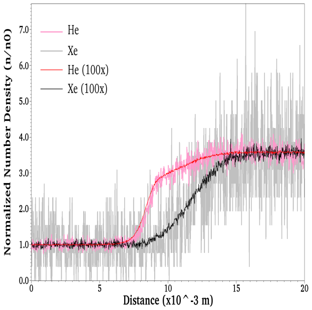


Instantaneous Baseline vs. 100x

1D Normal He:Xe Shock Test

- Mach 3.89 with He:Xe of 97:3 (i.e. Bird '94 Fig 12.35)
- Highlights Species Separation
- Separation Peak at $\rho_{He} \approx \rho_{Xe}$
- DSMC needs 33x He:Xe Macroparticles (From m_{Xe}/m_{He})
- Reduced Particle Count Introduces Error
- Error in Time Average at Baseline
- Instantaneous: Dramatic Noise in Xe

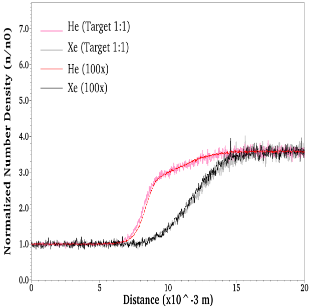
Noise Reduction via Variable Weights?



Instantaneous Baseline vs. 100x

1D He:Xe Shock with SWPM+Octrees

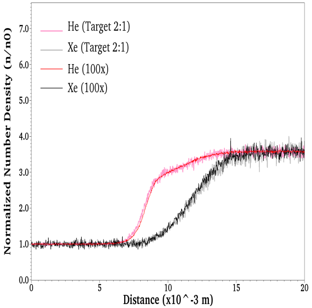
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable



100x vs. FDSMC 1:1

1D He:Xe Shock with SWPM+Octrees

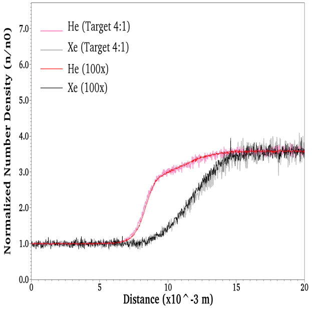
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 2:1

1D He:Xe Shock with SWPM+Octrees

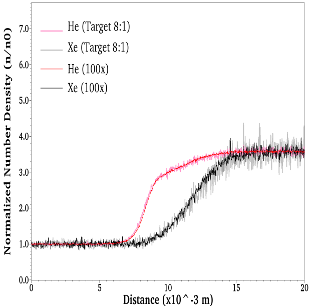
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 4:1

1D He:Xe Shock with SWPM+Octrees

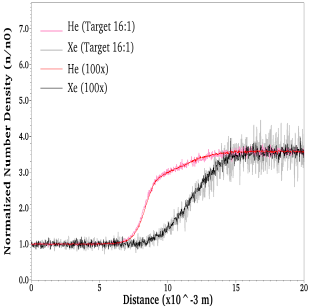
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 8:1

1D He:Xe Shock with SWPM+Octrees

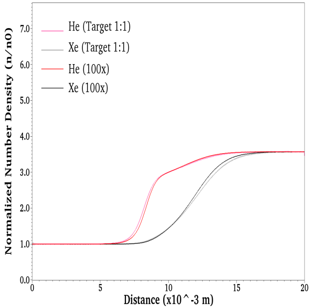
- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio



100x vs. FDSMC 16:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio
- Converged Error Finite! (1:1 Target)
- Error Source Still Unidentified...



Averaged 100x vs. FDSMC 1:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
- Direct Noise Control by Target Ratio
- Converged Error Finite! (1:1 Target)
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- Potentially Sensitivity to He Tails?
  -Merge Impacts Higher Moments
  -TBD Error vs. He-Noise Level
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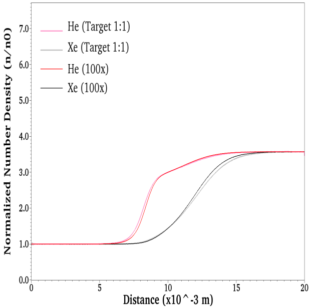
- Adaptation of SWMP Incorrect?
  -# of Collisions Sampled as WDF Varies?
  -Collision Pair Rule Wrong, $w_i \ll w_j$?



Averaged 100x vs. FDSMC 1:1

1D He:Xe Shock with SWPM+Octrees

- Xe Noise Controlled by 1:1 Target
- He:Xe Noise Comparable
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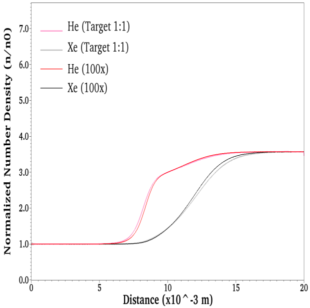
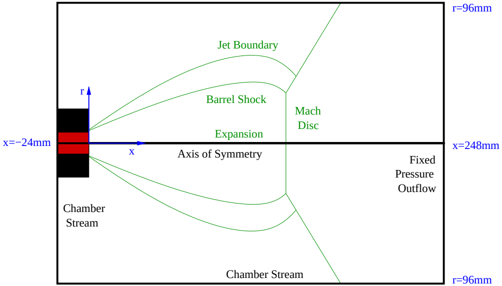
Error Identification in Future Work



Averaged 100x vs. FDSMC 1:1

- Helium-Argon Mixture
- Expanded through Nozzle to Vacuum
- *e*-Beam Concentration Measurements

Jet Flow Layout



Re=533

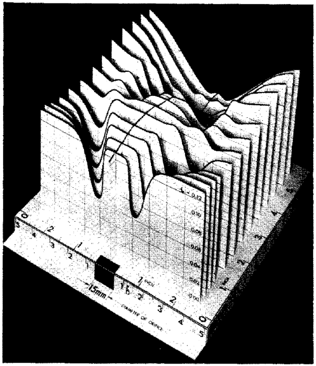
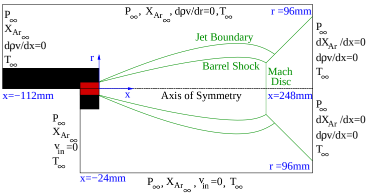


FIG. 11. Mole fraction of argon throughout the flow field of a free jet.

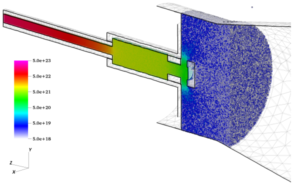
Case Tested in PhD & RGD27:

Continuum Boundary Conditions



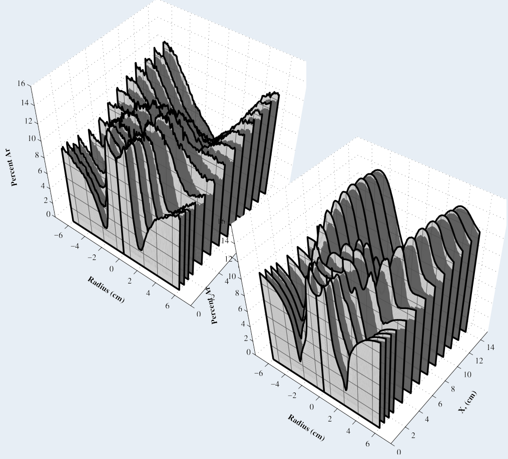
Monte Carlo Boundary Conditions

Surrogate for FRC Injection



Dynamic Range $\gg$ Shocks

Solution from DS2V



Solution from SPARTAN
(Navier-Stokes + Diffusion Velocity)

1. Wing Increases near Nozzle Edge

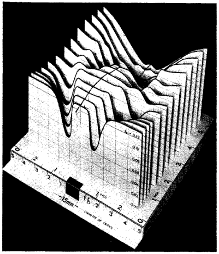
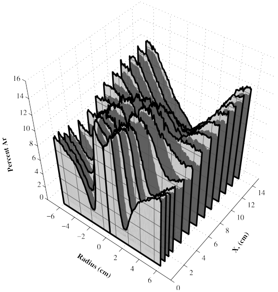
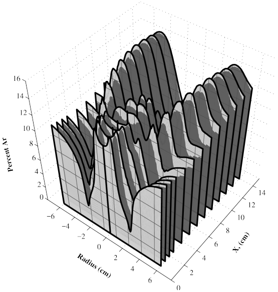


Fig. 11. Mole fraction of argon throughout the flow field of a free jet.

Experimental

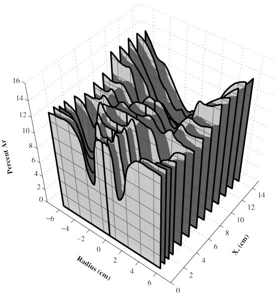


DS2V

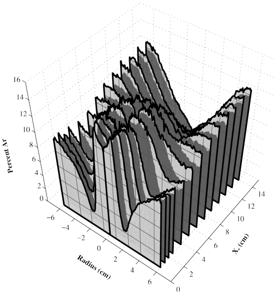


SPARTAN

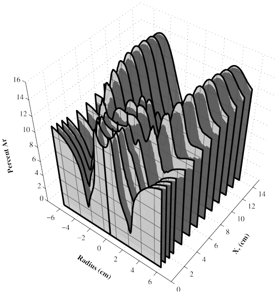
1. Wing Increases near Nozzle Edge



Experimental

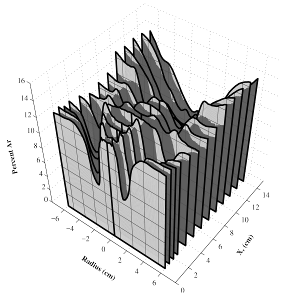


DS2V

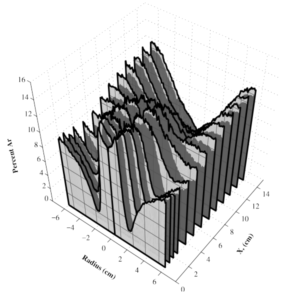


SPARTAN

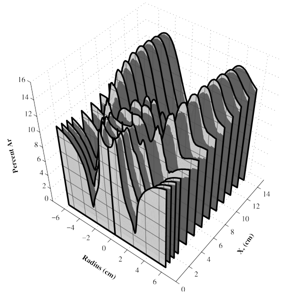
1. Wing Increases near Nozzle Edge
2. Lower Radial Boundary Edge Concentration



Experimental

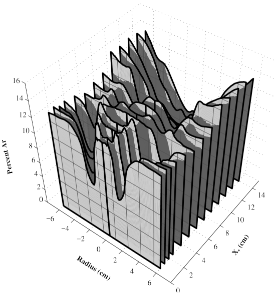


DS2V

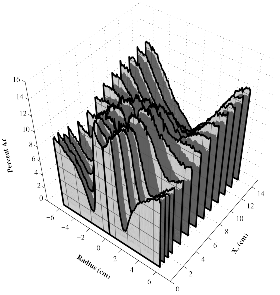


SPARTAN

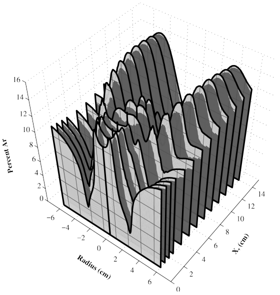
1. Wing Increases near Nozzle Edge
2. Lower Radial Boundary Edge Concentration
3. Deeper Jet Edge Concentration Drop



Experimental



DS2V



SPARTAN

Challenges for Jet in TURF

- TURF Naturally 3D Cartesian
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{||} v_{\perp}$-Quadtrees?)

Standard 3D DSMC

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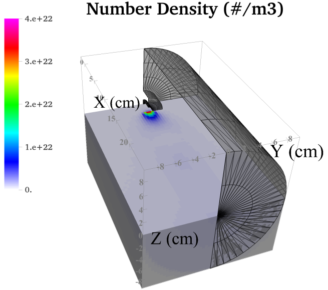
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{||}v_{\perp}$-Quadtrees?)
- Opted to Run Coarse Full 3D (Simplified Boundary Conditions)
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF

Standard 3D DSMC



Challenges for Jet in TURF

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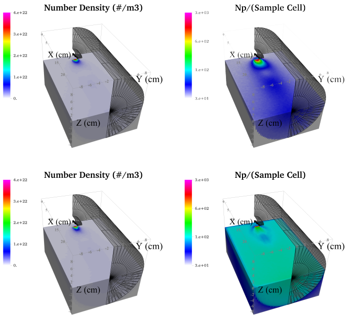
- Fractional DSMC Controls Np/Cell

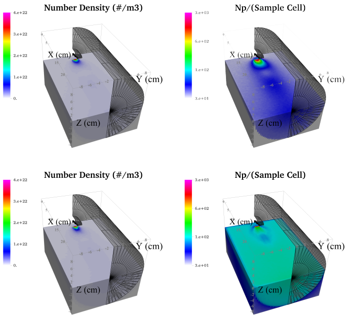
Standard 3D DSMC



Multi-Species Fractional DSMC

- TURF Naturally 3D Cartesian
- Considered 2D-Axisymmetric TURF
- Simple DSMC but Merge Complex (Conservation on $v_{\|} v_{\perp}$-Quadtrees?)
- Opted to Run Coarse Full 3D (Simplified Boundary Conditions)
- 3D Expensive at Tractable Resolution
- Added Collision Sub-Cells to TURF
- Fractional DSMC Controls Np/Cell
- Linear Density Obscures Results

Standard 3D DSMC



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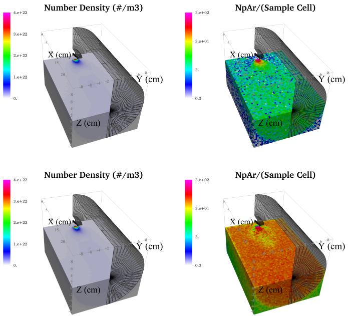

Multi-Species Fractional DSMC

Challenges for Jet in TURF

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X_{Ar} to RX-Plane $\rightarrow$ for Detailed Results...

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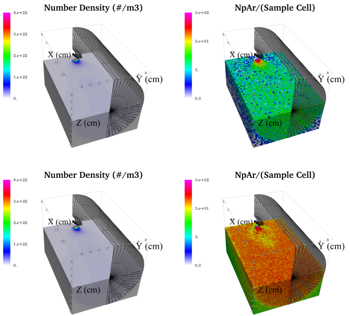

Multi-Species Fractional DSMC

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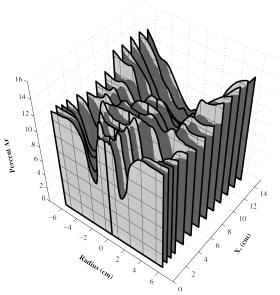
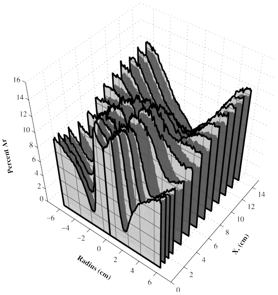
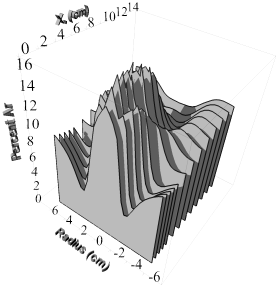


Experimental



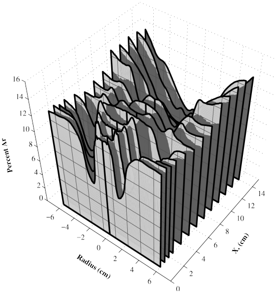
DS2V



TURF

1:1 - Collision:Sample

1. Standard DSMC Poor Results
2. 2x2x2 Collision Cell Improves Standard DSMC



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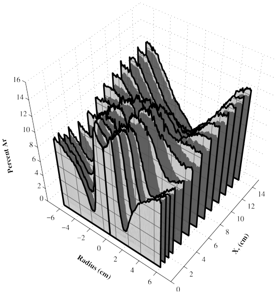

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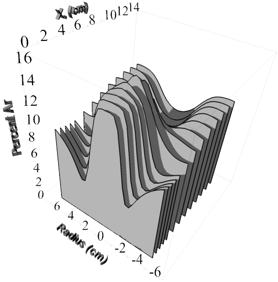
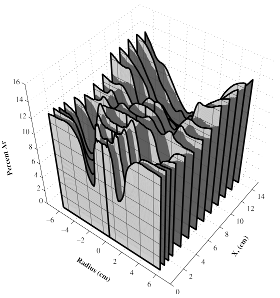


TURF

2x2x2:1 - Collision:Sample

1. Standard DSMC Poor Results
2. 2x2x2 Collision Cell Improves Standard DSMC
3. SWPM+Octree Significantly Better (2x2x2 Collision Cell)



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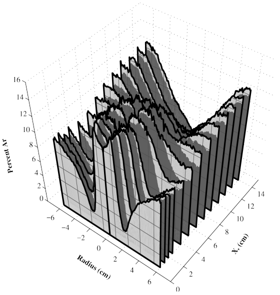

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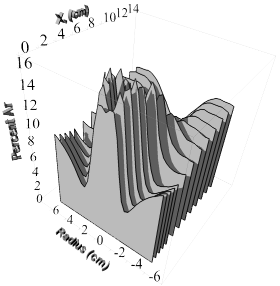

TURF

SWPM+Octree (2x2x2 Collision Cells)

The ∂f-Boltzmann for $f = f^{eq} + f^{dev}$

- ∂f - Concept Old
- How to make ∂f cheaper than full-f (Must adapt DOF Usage..?)

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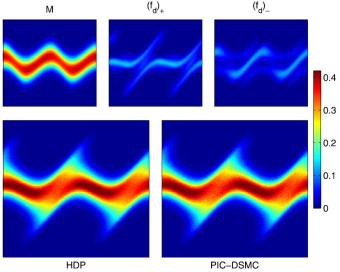
Strong Landau Damping



P-P:	v+,w+	$\to$	v'+,w'+
P-N:	v+,w-	$\to$	2v+,v'-,w'-
N-N:	v-,w-	$\to$	2v-,2w-,v'+,w'+
P-M:	M,v+	$\to$	M,w-,v'+,w'+
N-M:	M,v-	$\to$	M,w+,v'-,w'-
M-M:		$\emptyset$	

Yan, JCP 309 (2016) 18-36

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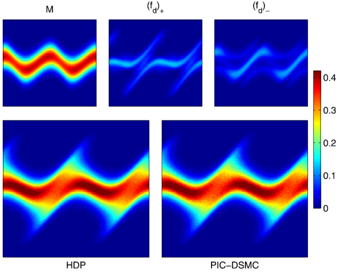

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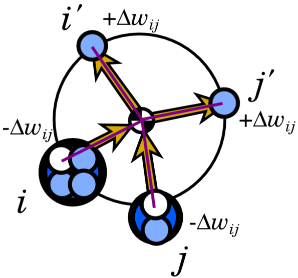
Stochastic Weight Particle Method (SWPM)



$w_i = w_i - \Delta w_{ij}$ & $w_j = w_j - \Delta w_{ij}$
$w_{(N_p+1)} = \Delta w_{ij}$ & $w_{(N_p+2)} = \Delta w_{ij}$

+2 Particles/Collision

RGD30

Future Directions: Hybrid ∂f

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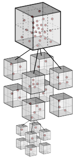
Octree ∂f-Boltzmann
Bin-to-Bin Collisions



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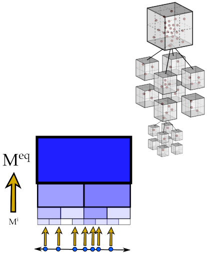

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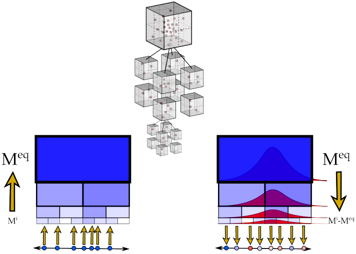

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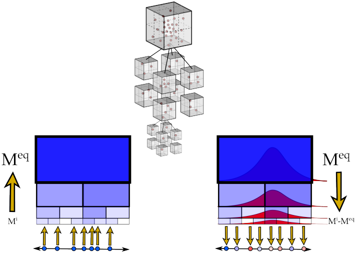

Sample Collisions using Δw: for P-P, P-N, N-N, P-M, N-M M-M:$\emptyset$

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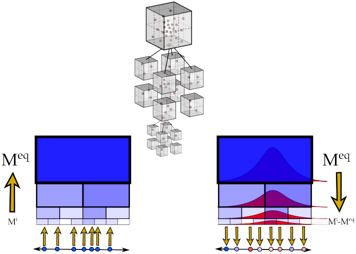

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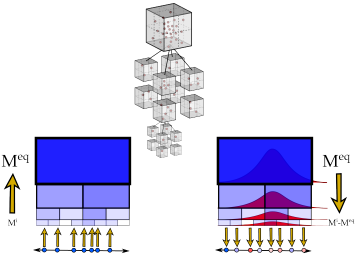
- Valid at Adaptive Tree Depths
- Entropy Estimate for DOF Distribution

Octree ∂f-Boltzmann
Bin-to-Bin Collisions



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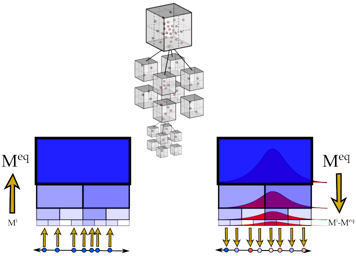

Sample Collisions using
Δw: for P-P, P-N, N-N, P-M, N-M
M-M:$\emptyset$
Combine with 2^6-Tree
XV $\rightarrow$ Multigrid Solves?

Conclusion

Current Results:

- SWPM+Octree Option for Variable Weight Mixture Collisions
- Multiple Octree Merge only Modification for Multi-Species
- Initial Verification vs. Standard Shock Cases
- Merge/Target Enables Direct Control of Noise
- Unidentified Systematic Error with 1:1 Target
- Initial Testing on 3D Mixture Expansion Better with SWPM+Octree

Future Efforts:

- Additional Investigation of Error Source for Disparate Weights
- Improved Merge/Control of Tails
- Apply to Reacting Flow
- Adaptation for δf

Thank You

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Any opinions, finding, and conclusion or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the United States Air Force.

Questions?